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LLNL-TR-648450

HPC4Energy Wrapup Report - LDRD 12-ERD-074

E. Dube

January 14, 2014

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

LLNL-TR-648450

Hpc4energy Wrap up report

October, 2013

Lawrence Livermore National Laboratory

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Improving Simulations of Advanced Internal Combustion Engines

hpc4energy incubator wrapup

October 2, 2013

Robert Bosch LLC

in collaboration with

Lawrence Livermore National Laboratory

Robert Bosch

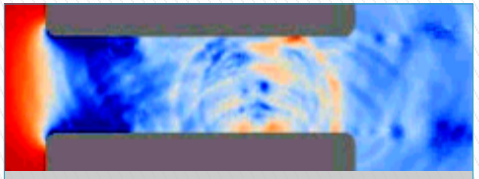
Est.	Employees[1]	Sales (USD/yr)[1]
1886	302,500	$71.3 billion
1906	22,500	$9.8 billion

- **“Invented for Life” Innovation**
  - 38,500 R&D associates (2,500 in North America)
  - Global R&D expenditure: $5.8 billion USD[1]
  - A world leader in patent applications (4,126 in 2011)
    - Ranked No. 1 in Germany, No. 5 in world

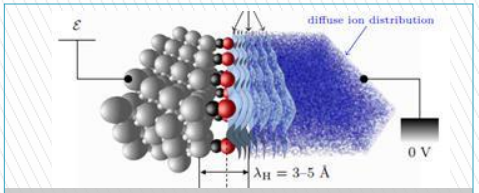
Research at Bosch

Automotive Technology	
Industrial Technology	
Consumer Goods and Building Technology	

- **High Performance Computing at Bosch**
  - Recent investment in terascale facilities (~100 TFLOP)
  - HPC development recognized as key for component development in energy sector
    - Energy Conversion: Materials optimization; multi-scale, multi-physics coupled simulations
    - Energy Storage: Materials discovery; Cell physics



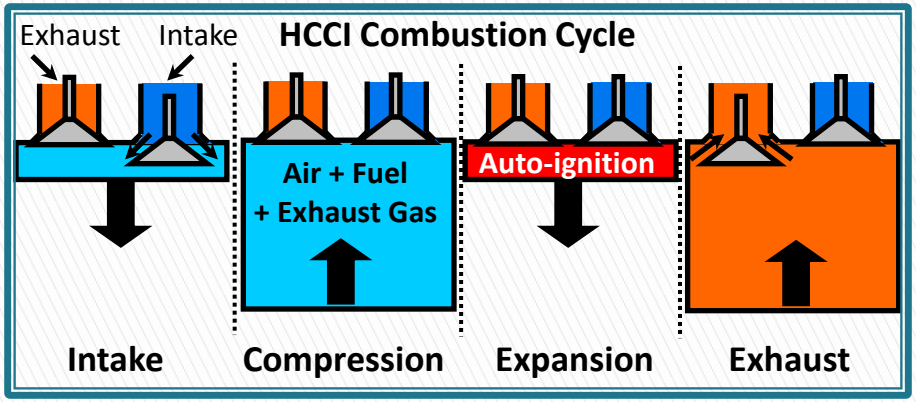
LES: Cavitation

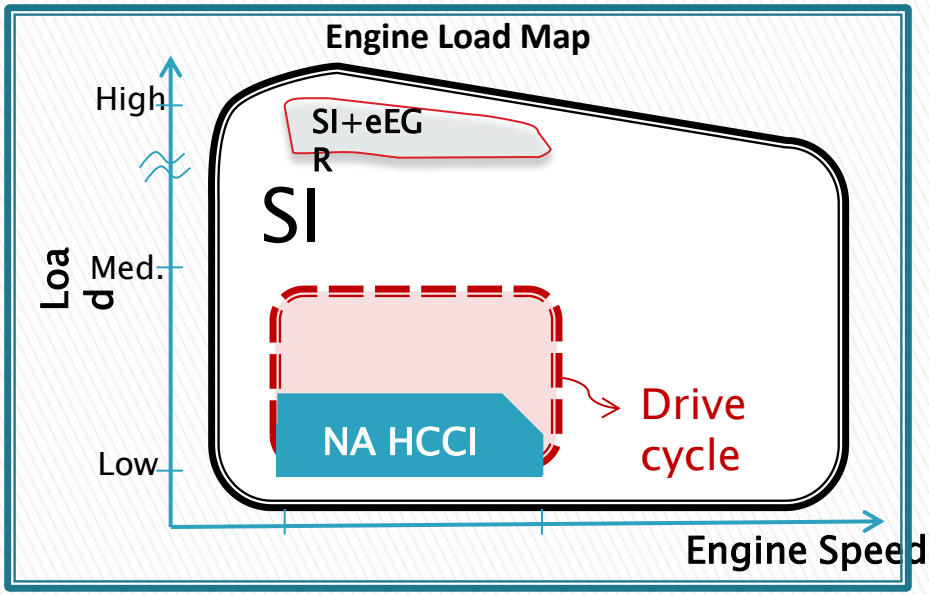


Ab-initio Simulations

Advanced Internal Combustion Engines

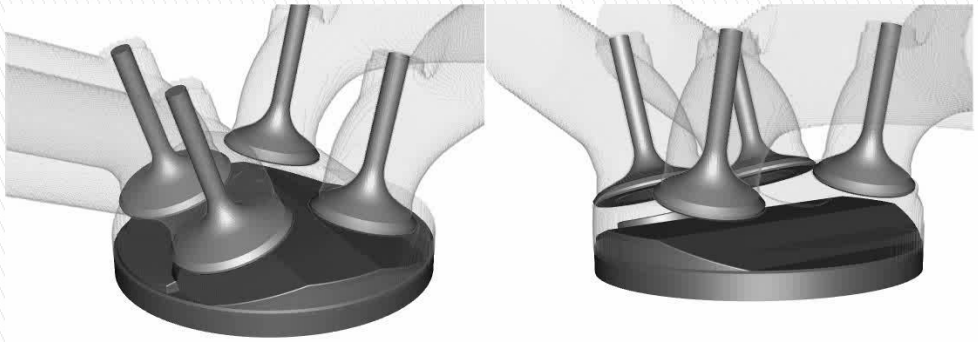
- **Advanced Combustion Concepts**
  - High efficiency (+30%), low emissions
  - Advanced control algorithms required for robust operation
  - Multi-mode operation enables optimal operation over load map
- **Project Goals**
  - Understand the transient dynamics of switching between SI and HCCI combustion modes
  - Aid the development of effective control strategies for multi-mode combustion engines





Advanced Internal Combustion Engines

- **Modeling Approach**
  - Large Eddy Simulation (LES) of engine transition
  - Structured explicit compressible code developed with Stanford U.
  - Run on 1000-2000 core
  - 1.5-2 mio CPU-hrs/transition
- **Benefit of hpc4energy**
  - LES of transition feasible in timeframe relevant to make impact
    - 70% reduction in time/cycle
  - High fidelity critical to aid development of physics-based controller



Key Results

- CAIO Combustion Code Run for SI to HCCI transition
  - 4 days/engine cycle on 2000 cores
  - Ran several different multi-cycle simulations, order 10^7 CPU-hours utilized
- Evaluated CAIO code at higher resolution than previously possible
  - “Conditions under investigation”

Value added by HPC/LLNL collaboration to the Company

- Evaluated CAIO code at not previously obtainable levels of resolution
- Discovered limitations of CAIO combustion simulations at high resolution
- Learned that HPC is a valuable tool, but need codes better designed for large scale simulation

Value added by collaboration to LLNL

- Gained insight into Bosch development process and needs
- Learned how to effectively and efficiently collaborate with industry in HPC
- Set framework for future collaboration with other partners (GE, Cummins, etc.)
- Continuing engagments in non-combustion activites

"Evaluation of Robust Unit Commitment"

hpc4energy incubator wrap-up

October 1st, 2013

LLNL: Vera Bulaevskaya, Alan Lamont, Liang Min, Deepak Rajan, and Barry Rountree

ISO NE: Eugene Litvinov and Jinye Zhao

"ISO New England"

in collaboration with

Lawrence Livermore National Laboratory

Overview of ISO New Engla

- 550 employees
- Three core responsibilities
  - Ensure the day-to-day reliable operation of New England's bulk power generation and transmission system;
  - Oversee and ensure the fair administration of the region's wholesale electricity markets; and
  - Manage comprehensive, regional planning processes.
- Administer markets ranging from $5-$11 billion annually
- Operate 8,000 miles of HV transmission lines; 13 interconnections to electricity systems in New York and Canada

- Interests in High Performance Computing
  - Internal production system using PSSE and TARA with Enfuzion in Transmission Planning and Operations Planning studies
  - Pilot project with Cycle Computing to use TARA and

    Condor job scheduler at Amazon EC2
  - R&D project with EPRI on GPU based power flow application

Evaluation of Robust Unit Commitment

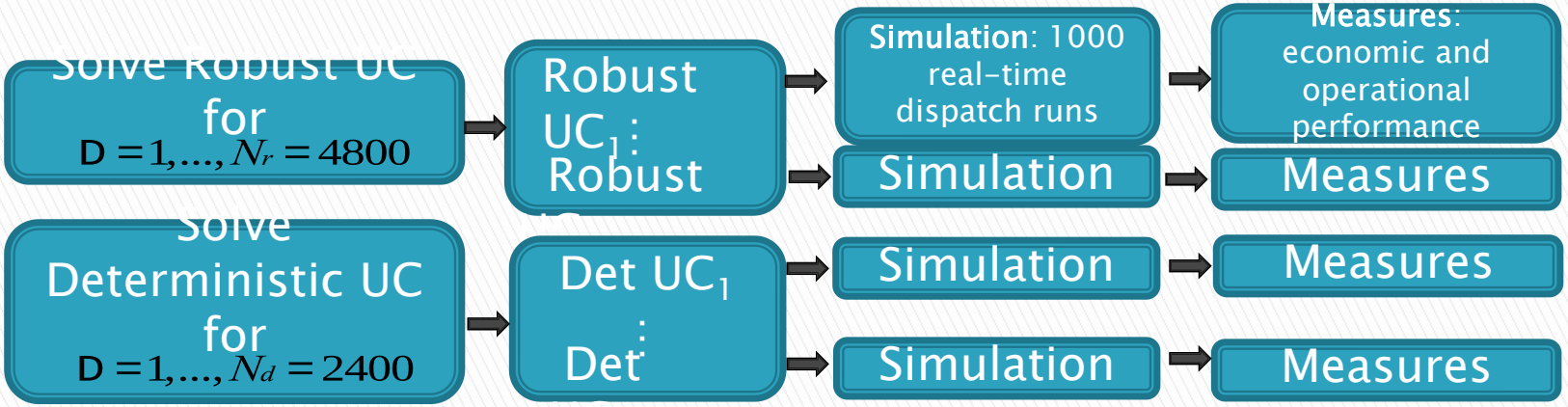
- Benefits to the energy sector:
  - Efficient computation enables ISO NE to perform more accurate and more comprehensive evaluation of the robust UC.
  - Optimized generator operation and improved market efficiency.
- Project goal:
  - Compare the robust approach with the deterministic approach by running a large number of Monte Carlo simulations.
  - Evaluate the operational and economic benefits.
  - Identify the optimal conservatism level of the robust approach.

Key Results

Time to solve 7200 UC and 7.2 million ED problems decreased from 600 days to 9.5 hours

- Generate random samples for simulations
  - Number of historical data is small
  - Use the "cluster method" to create clusters of samples
- Solve robust UC problems
  - Multiple robust problems can be solved at the same time.

    1000 ED runs for each robust UC
    1 robust UC and 1000 ED runs per core
    4800 cores used for 4800 robust UC and 4.8 million ED runs



Value added by HPC/LLNL collaboration to ISO NE

- HPC can efficiently run millions of simulations, which is impossible to be achieved by the computing capability of ISO NE.
- Simulations yield more statistically significant results.
- Efficient computation enables ISO NE to perform more accurate and more comprehensive evaluation of the robust UC.
- LLNL provides expertise in HPC and statistics.

Value added by collaboration to LLNL

- ISO-NE keeps promoting LLNL's value. This helps us build reputation in grid area.
- Engaging with ISO NE helps us understand better the R&D needs at RTO/ISO community.
- ISO NE and LLNL are co-authoring an IEEE paper.
- We were approached by GAMS to scale up the simulation to 1 million ED runs for each UC.

Improving Models for Spray Breakup in Liquid Fuels Combustion

hpc4energy incubator wrap-up

October 2, 2013

GE Global Research

in collaboration with

Lawrence Livermore National Laboratory

Cornell University

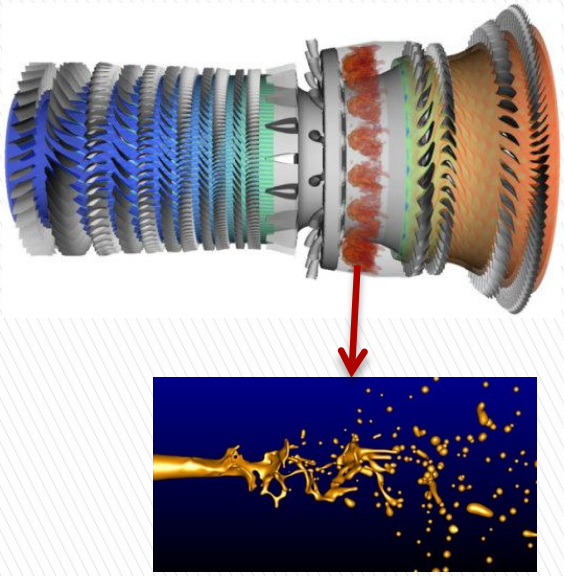
Arizona State University

GE Global Research: Spray Breakup

GE jet engine design issues

- Efficiency, reliability, durability, minimizing pollutant formation
  - Little current use of HPC
  - Still designing with older paradigms & methods

Jet Turbine & Combustor



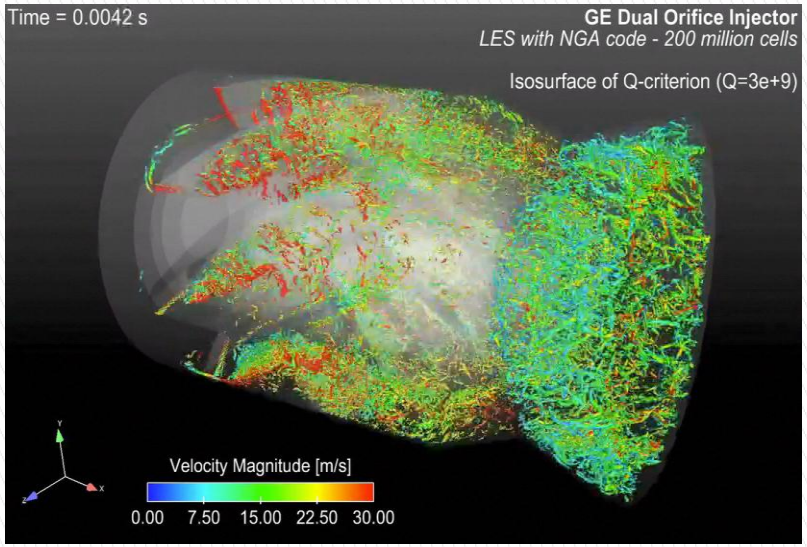
Liquid Fuel Breakup

Project goal

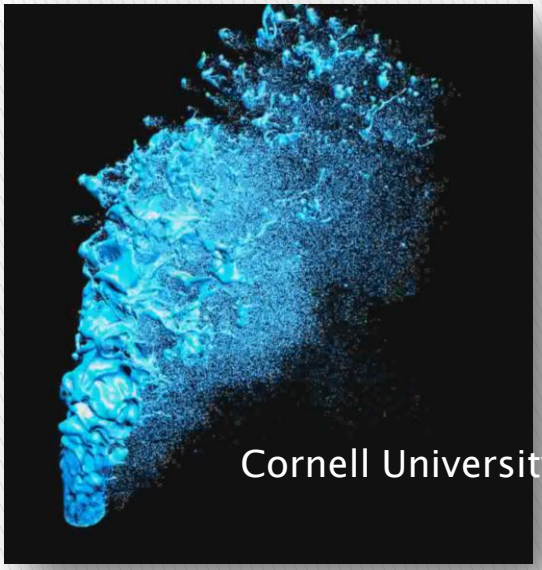
- HPC to study realistic fuel injector designs
  - Evaluate computational approaches to model complex geometries
  - Identify HPC needs for predictive spray breakup simulations

Key Results: Liquid Jet in Cross Flow

Prior Simulations: complex geometry but low fidelity models



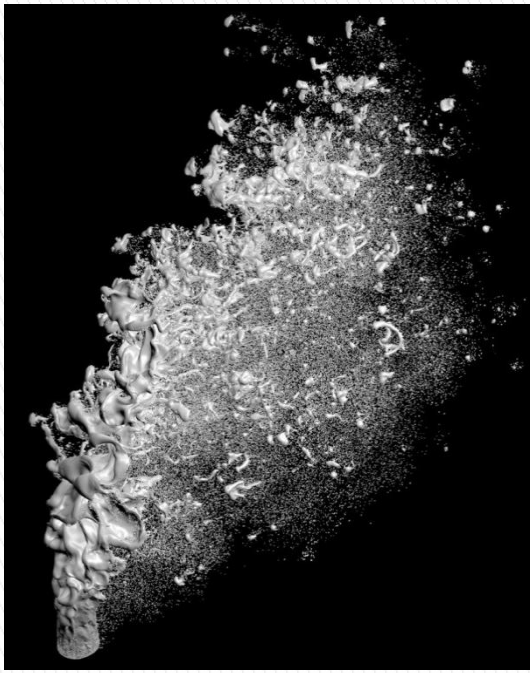
HPC4Energy simulations



- Simulations capture physics consistently with experiment
- Richer physics with better models and denser mesh

Value added to GE Global Research

- Simulation sizes not normally run in an industrial setting
- Insight into better models for JIC in near-injector and dense spray regions
- Potentially fewer, better designed experiments to shorten design and development process
- Provides evidence for value of HPC within company



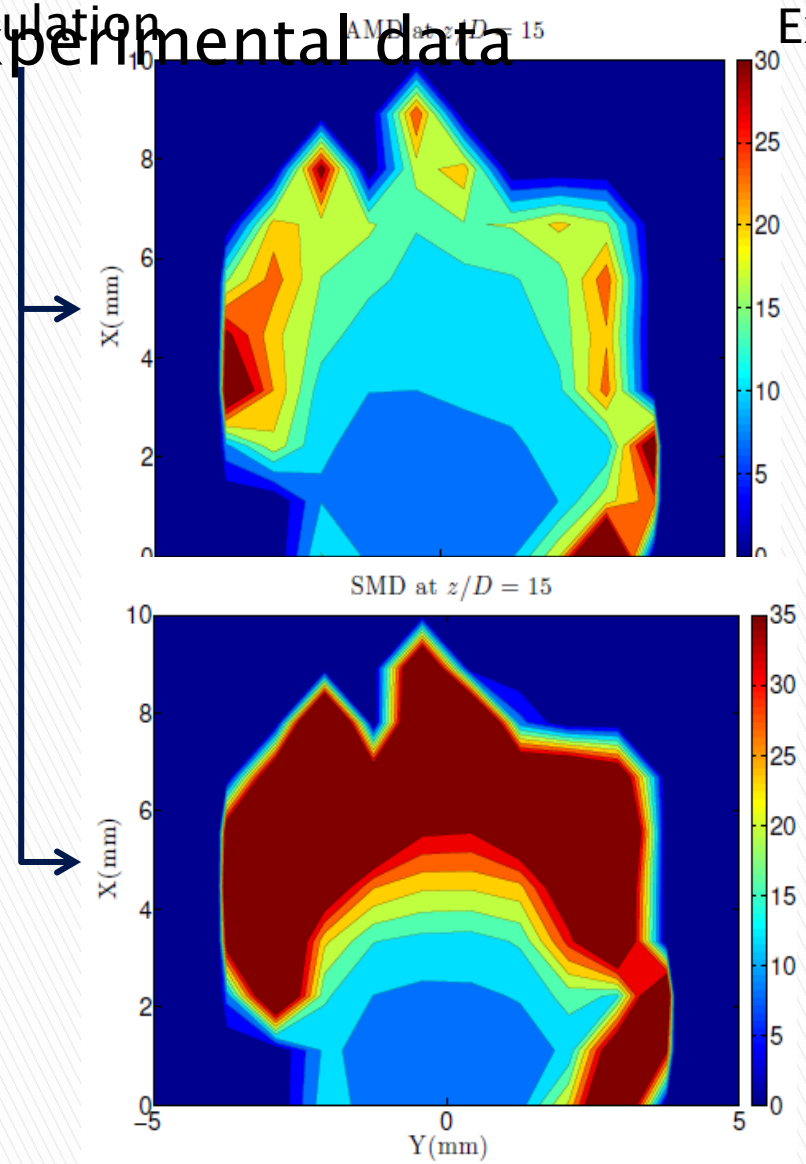
Value added to LLNL

- Perspective of industry applications involving spray breakup, and what is the current state-of-the-art.
- Access to source algorithm allows us to "pull apart" and learn about these state-of-the-art numerical techniques, and continuing collaboration with academia
- Codes are ported to HPC machines, configured for +10K core runs, now available for LLNL work through TASC (***tasc.llnl.gov***)
- **Future**: Other multiphase flows at LLNL, e.g., Advanced Rocket-Engine Design (DARPA)

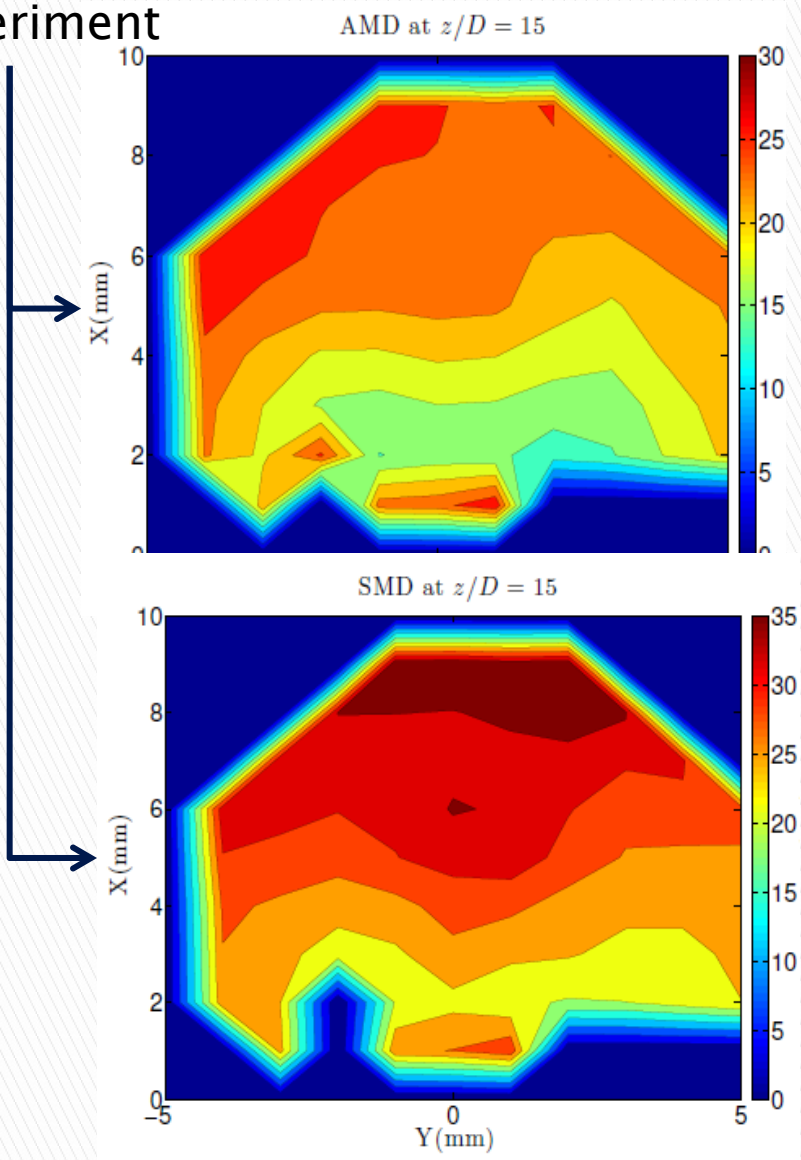
BACK UP SLIDES

Validation of JIC numerical simulations with experimental data

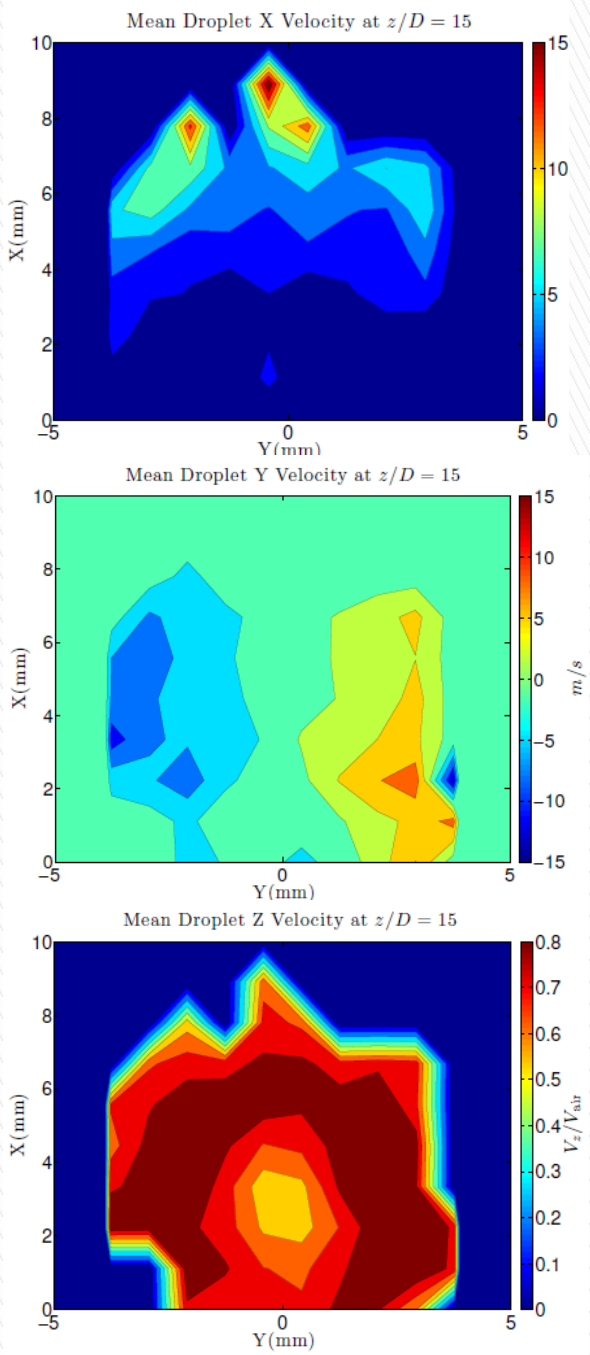
Simulation



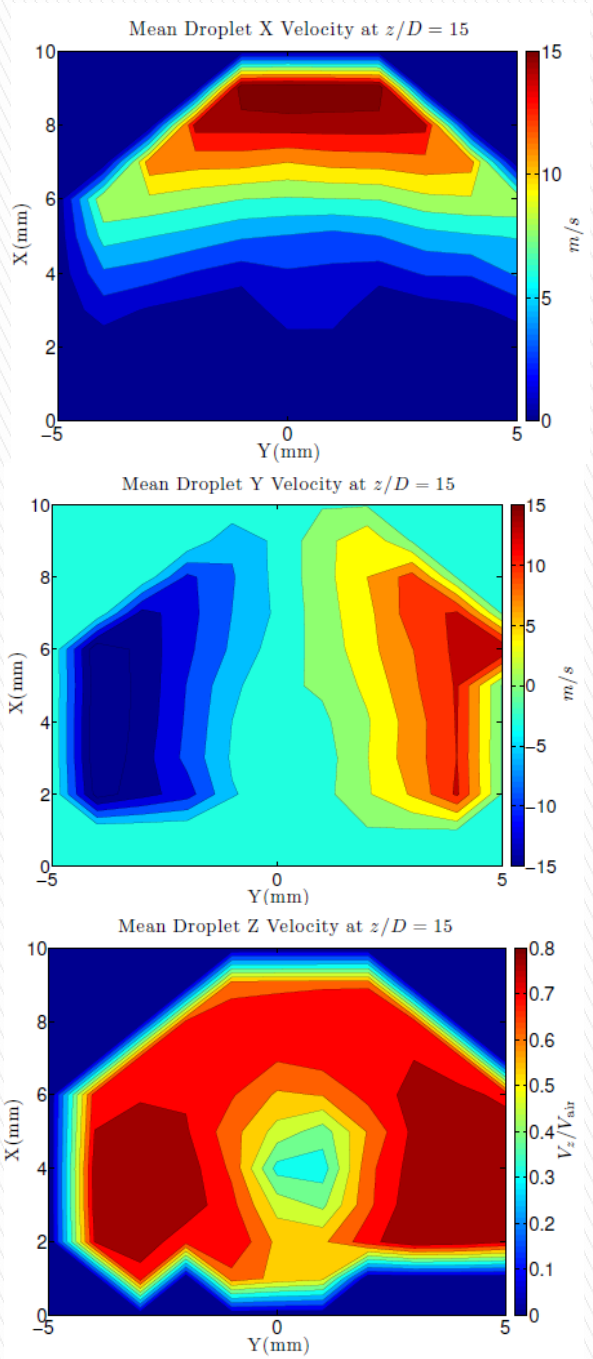
Experiment



Simulation



Experiment



Comparison of drop velocities from JIC numerical simulations with experimental data

- Encouraging match with experimental data
- Simulation needs more time averaging to smooth out statistical error

Improving Thermal Spallation Drilling with HPC Simulations

hpc4energy incubator wrapup

October 2, 2013

Potter Drilling

in collaboration with

Lawrence Livermore National Laboratory

Potter Drilling

POTTER DRILLING
Drilling Technology for Clean Energy

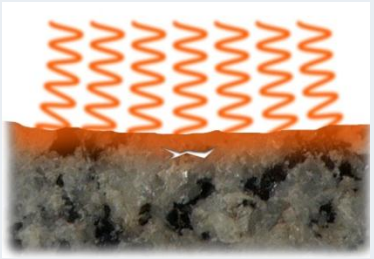
- Cleantech start-up
  - Developing innovative drilling and rock excavation technologies for revolutionary performance in hard rocks
  - Geothermal, oil & gas, mining
  - Only have access to workstation-scale CFD and FEA

- Need HPC to complement and reduce empirical development
  - High cost and long time associated with field trials
  - Challenge of observing/measuring downhole process
  - Determining changes in process parameters for differing rock types
  - Extrapolating to greater depths and conditions not feasible for testing

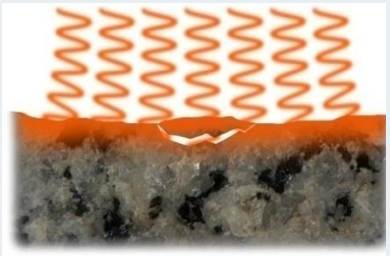
Thermal Spallation: An Effective Way to Excavate Hard Rock

POTTER DRILLING
Drilling Technology for Clean Energy

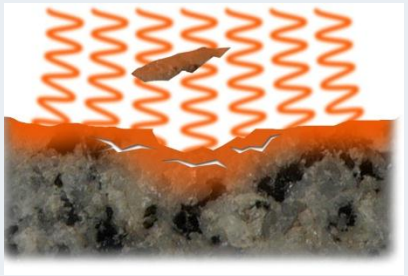
1. Intense heat creates high stress at the rock surface



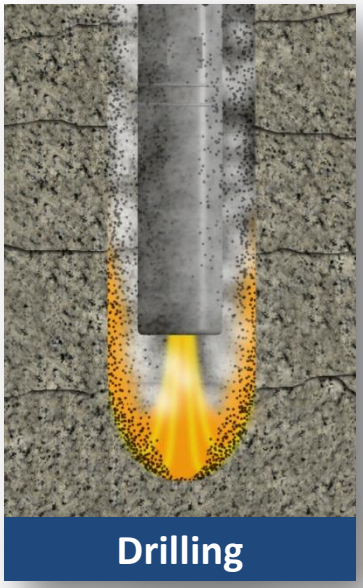
2. Micro-fractures initiate at flaws or mineral boundaries



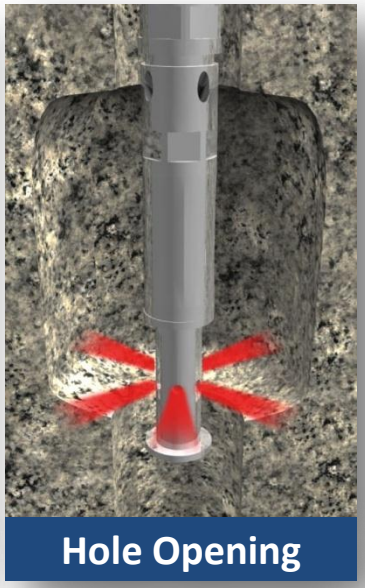
3. To relieve stress, spall is ejected, exposing fresh surface



Non-contact technology removes hard rock wherever heat is applied



Drilling



Hole Opening

Project Description

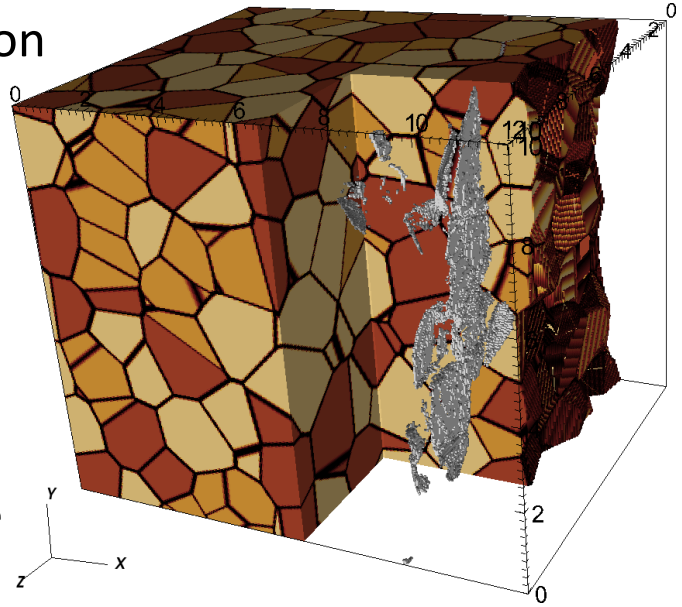
POTTER DRILLING
Drilling Technology for Clean Energy

- HPC for Thermal Spallation Drilling
  - Potential to decrease cost of drilling hydrothermal wells by up to 25% (value of $1M/well)
  - Net increases in geothermal productivity by at least 2x (value of $5-7M/well)
  - Enables more widespread Engineered Geothermal Systems (EGS)
  - Applications to oil & gas: decreases hard rock drilling costs, increased well productivity, EOR, non-hydraulic fracking, and more.

- Scope of Work
  - Conduct a detailed parametric analysis of the factors impacting thermal spallation of hard basement rocks.
  - Extract the necessary parameters (spall sizes, critical flaw distributions and critical stress thresholds etc.) needed to validate parametric models

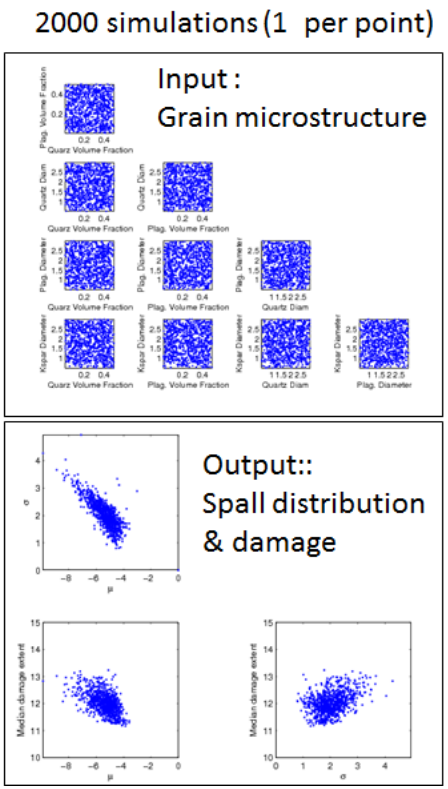
Results

- Finished Stage 1 & 2 simulations
  - 2D: Completed over 7000 simulations
    200K CPU-hrs; **72** processors per simulation
  - 3D: Completed 50 simulations
    500K CPU-hrs; **1020** processors per simulation
- Five sets of 2D parametric runs have been completed and analysed
  - Examined: borehole conditions, microstructural properties, thermal and mechanical properties.
  - Determined factors most crucial to damage extent and spall size.
  - Results used to constrain 3D parameter space and reduce number of runs.



Value Added by *hpc4energy* Collaboration

- Providing valuable insights into the actual mechanism for spall formation
- Identifying most critical parameters for optimizing process
- Will allow for extrapolation to depths and conditions not feasible by empirical approach
- HPC resources not otherwise available to small or start-up companies



Value Added by Collaboration to LLNL

- Better understanding of effective strategies and challenges when working with small businesses
- Promotion of LLNL's HPC capabilities to the geothermal and drilling communities
- Implementation and validation of a new GEODYN-PSUADE interface to control simulation runs and analysis.

“Improving PSLF Simulation Performance and Capability”

hpc4energy incubator wrapup

October 2, 2013

in collaboration with

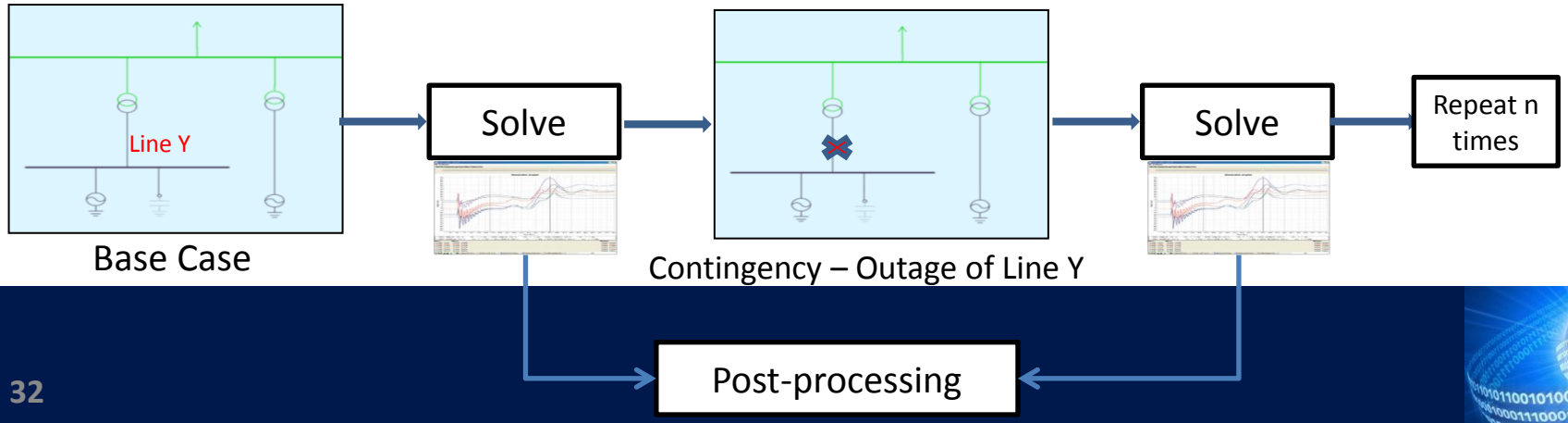
Lawrence Livermore National Laboratory

GE Energy Overview

GE Energy

- ~$45 billion/yr
- ~100,000 employees
- Software ~$3B
- Main business segments
  - Energy Management
  - Oil and Gas
  - Power and Water

- GE Concorda suite of tools
  - Planning and simulating electric power grids
  - Assessing economic performance
  - Evaluating generation reliability.
  - Deployed to 130+ companies
- PSLF transmission planning component
  - Steady state and dynamic analysis
  - Study impacts of system events
- The hpc4energy project focused on contingency analysis performance
  - Scaling
  - Computational efficiency
  - Current runtimes are hours to days

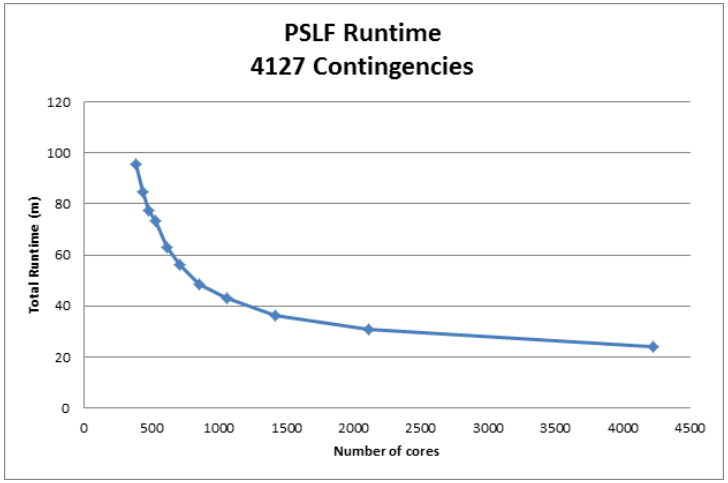


Benefits to Industry

- Improve ability to identify potential major system reliability concerns
- Improve evaluation of emerging clean energy technologies
- More accurate models with greater than 150,000 buses
- Focus on results analysis and less time on performing analysis has a direct financial benefit for utilities

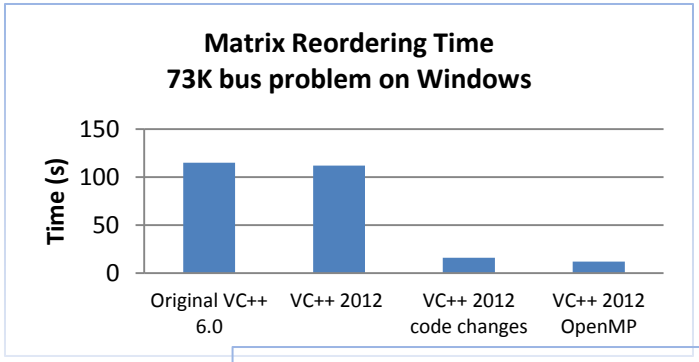
Key Results

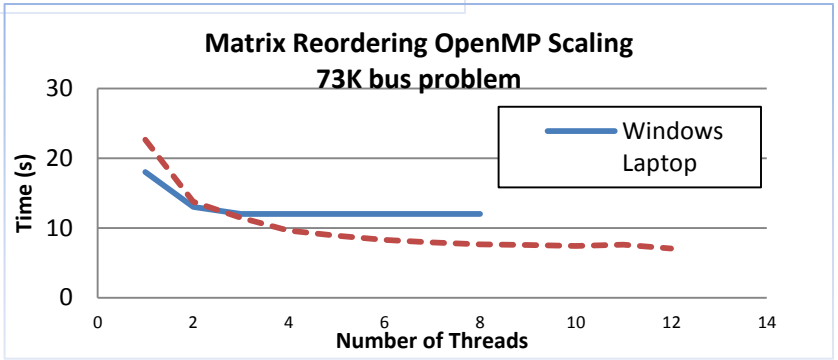
- Parallel execution of contingencies enables larger more complete studies
- Large number of contingencies (4,217); current norm is 100's



Reduced runtime from 23.5 days to 23 minutes

- Significantly improved matrix reordering algorithm solution times through optimization and threading





Reordering speedup of 9.6 times on Windows and 7.2 times on Linux

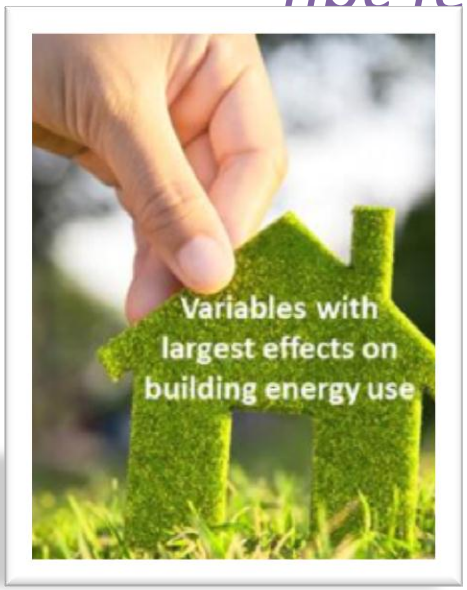
Value added by collaboration to LLNL

- Built relationships and credibility
- Demonstrated how LLNL HPC expertise can be applied to an industry application
- New domain for applying LLNL developed solvers
- Technical experience and knowledge
  - Application used by CA utilities
  - Looking into a power system modeling application
  - Porting Windows applications to HPC
  - Running thousands of instances of an application

“Building System Models to Enable Deep Energy Retrofits”

hpc4energy incubator wrap up

October1, 2013



in collaboration with

Lawrence Livermore National Laboratory

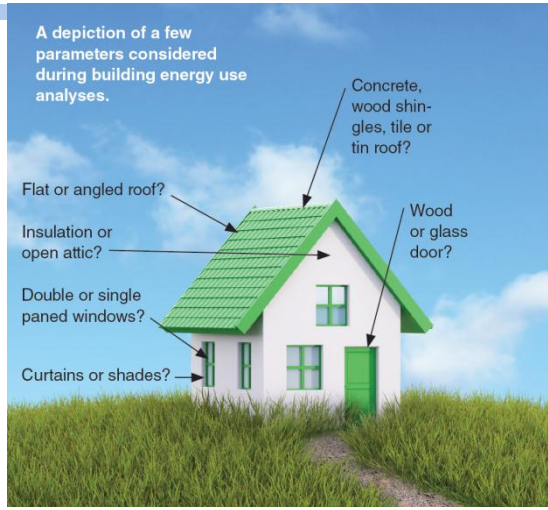
UTRC Research

United Technologies Research Center

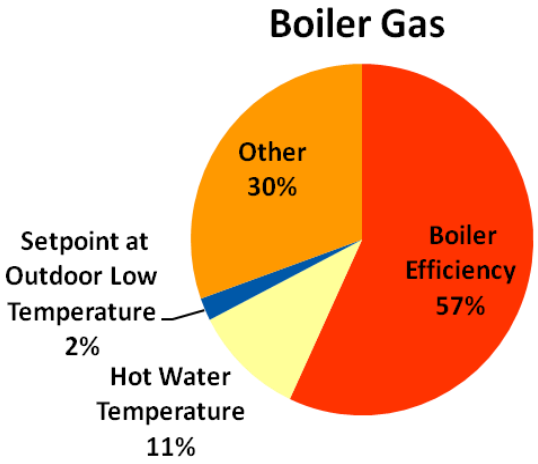
- $60B in revenue (UTC), 1,000 employees (UTRC)
  - *UTC: Carrier, UTC Aerospace, Otis, Pratt & Whitney, Sikorsky Aircraft, UTC Fire & Security*
  - UTRC: Research arm of UTC
- UTRC: An unclear HPC investment strategy
  - Currently use computing at giga-scale
  - UTRC, Sikorsky, others….
- Buildings use 40% of energy in the US annually
  - Buildings typically use up to 30% than designed

Key Results

- Building Energy Simulation
  - Identify most impactful parameters
  - Speed up process
  - ROM, UQ via PSUADE



- UTRC ran over 10,000 runs on Sierra
  - Each run used 1,000 cores
  - Processing time reduced by a factor of 60



- Only 50 of 917 parameters impacted the simulation
- Model calibration: error reduced to 5%

Value added by HPC/LLNL collaboration to the Company

- Project improvement:
  - Reduced time
  - Expanded parameter set
- HPC is a great resource for UTC
- LLNL collaboration can help improve their computational, analytical, and algorithmic capabilities

Value added by collaboration to LLNL

- Better understanding of UTC
- Established expertise in the Building Simulation domain
- A real champion in HPC and LLNL from UTC
- Expansion of LLNL in EEB Hub, leading to EERE projects